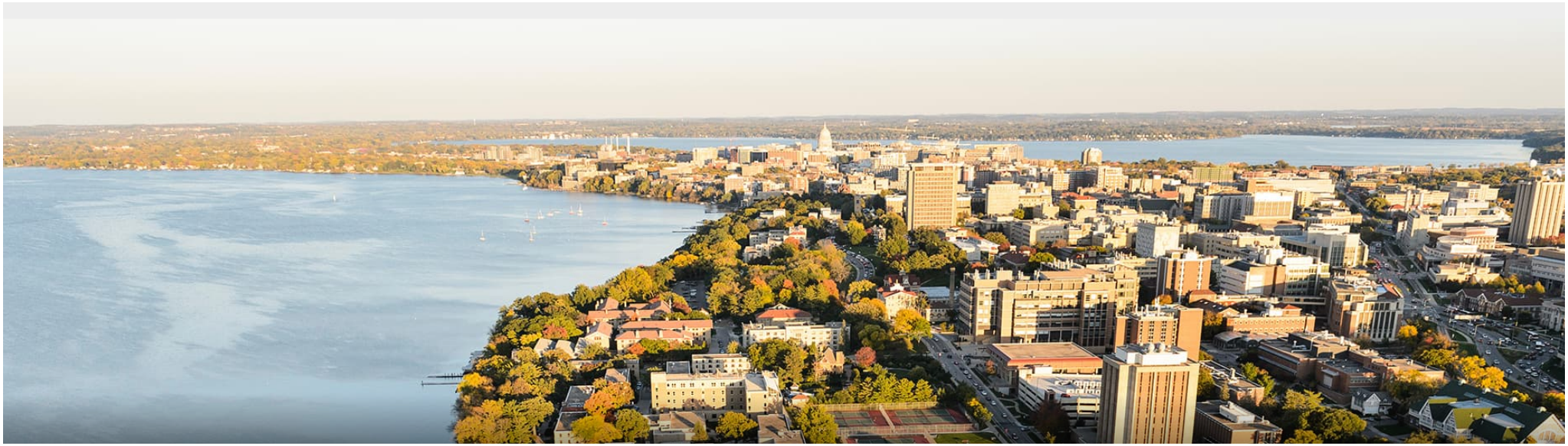


CS 760: Machine Learning
Intro to Learning Theory

Ilias Diakonikolas

University of Wisconsin-Madison

Nov. 22, 2022

Announcements

- **Logistics**:
  - HW 6 due after Thanksgiving.
  - Happy Thanksgiving! Enjoy break.
- Class roadmap:

	PCA Review & Learning Theory
	RL I
	RL II
	RL III
	Fairness & Ethics

Outline

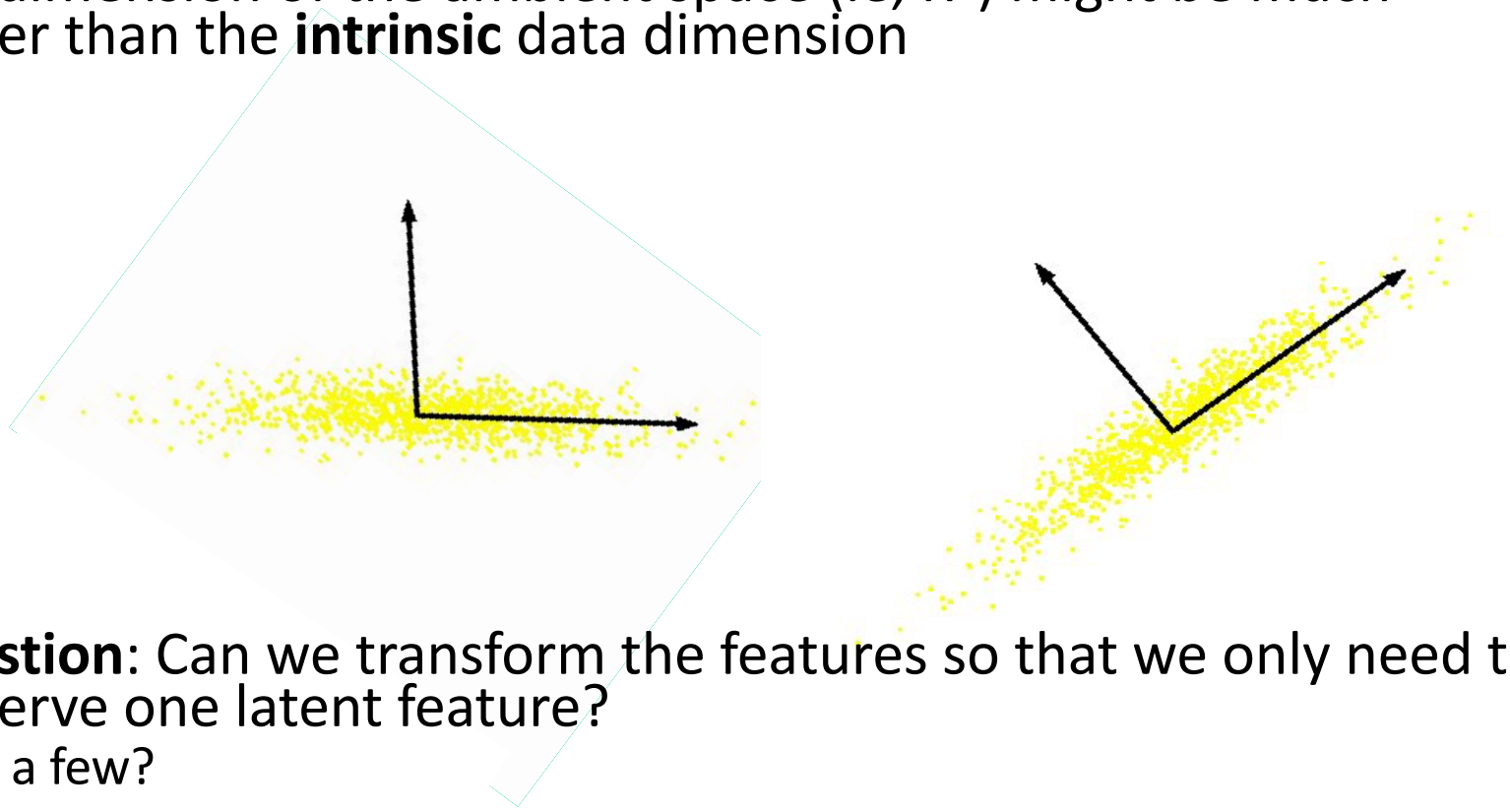
- **Review & PCA**
  - Intuition, operation, interpretations, compression
- **Intro to Learning Theory**
  - Error decomposition, bias-variance tradeoff
- **PAC Learning Framework**
  - Definition, intuition, sample complexity bounds

Outline

- **Review & PCA**
  - Intuition, operation, interpretations, compression
- **Intro to Learning Theory**
  - Error decomposition, bias-variance tradeoff
- **PAC Learning Framework**
  - Definition, intuition, sample complexity bounds

PCA Intuition

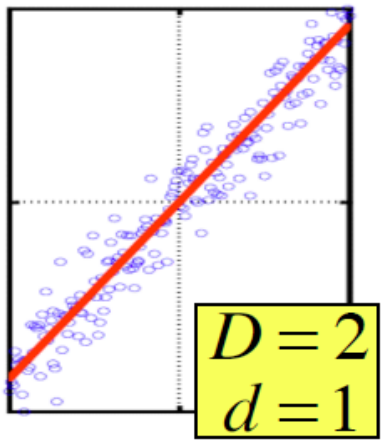
- The dimension of the ambient space (ie, R^d) might be much higher than the **intrinsic** data dimension

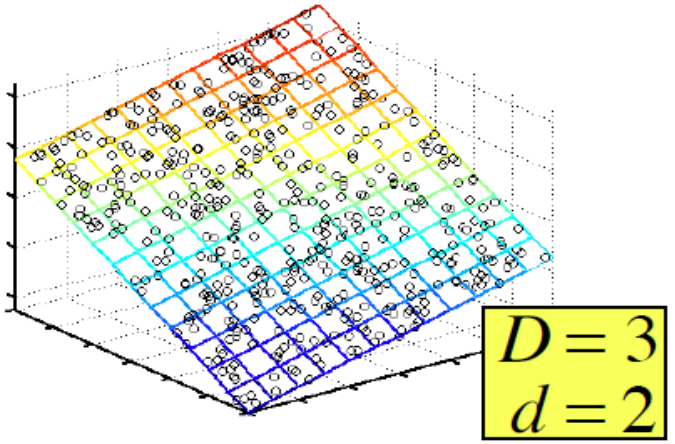


- **Question**: Can we transform the features so that we only need to preserve one latent feature?
  - Or a few?

PCA Intuition

- Some more visualizations

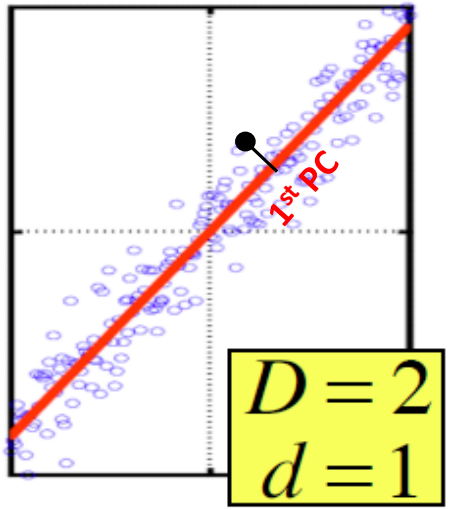




- In case where data lies on or near a low d-dimensional linear subspace, axes of this subspace are an effective representation of the data.

PCA: Principal Components

- **Principal Components (PCs)** are orthogonal directions that capture most of the variance in the data.
  - First PC – direction of greatest variability in data.
  - Projection of data points along first PC discriminates data most along any one direction



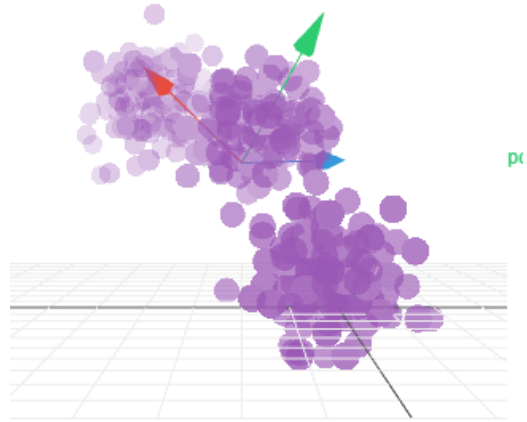
PCA: Principal Components and Projection

- How does dimensionality reduction work? From *d* dimensions to *r* dimensions:
  - Get
  - Orthogonal!

$$v_1, v_2, \ldots, v_r \in \mathbb{R}^d$$

- Maximizing variability
  - Equivalent to **minimizing reconstruction error**

- Then project data onto PCs → d-dimensional



Victor Powell

PCA First Step

- First component,

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{n} \langle v, x_i \rangle^2$$

- Same as getting

$$v_1 = \arg\max_{\|v\|=1} \|Xv\|^2$$

PCA Recursion

- Once we have *k-1* components, next?

$$\hat{X}_k = X - \sum_{i=1}^{k-1} X v_i v_i^T$$

Deflation

- Then do the same thing

$$v_k = \arg \max_{\|v\|=1} \|\hat{X}_k w\|^2$$

PCA Interpretations

- The v's are eigenvectors of XX^T **(Gram matrix)**
  - We'll see why in a second

- XX^T (proportional to) sample covariance matrix
  - When data is 0 mean!
  - I.e., PCA is eigendecomposition of sample covariance

- Nested subspaces *span(v1), span(v1,v2)*,…,

PCA Interpretations: First Component

- Two specific ways to think about the first component
- **Maximum variance direction**
  - What we saw so far

$$\sum_{i=1}^{n} (\mathbf{v}^T \mathbf{x}_i)^2 = \mathbf{v}^T \mathbf{X}\mathbf{X}^T \mathbf{v}$$

- **Minimum reconstruction error**
  - A direction so that projection yields minimum MSE in reconstruction

$$\sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T \mathbf{x}_i)\mathbf{v}\|^2$$

PCA Interpretations: Equivalence

- Interpretation 1.

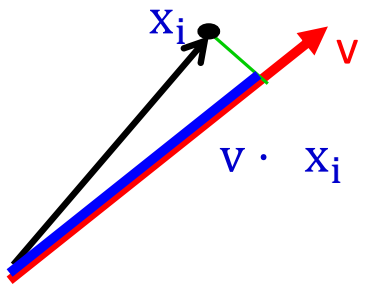
Maximum variance direction

$$\sum_{i=1}^{n} (\mathbf{v}^T \mathbf{x}_i)^2 = \mathbf{v}^T \mathbf{X}\mathbf{X}^T \mathbf{v}$$

- Interpretation 2.

Minimum reconstruction error

$$\sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T \mathbf{x}_i)\mathbf{v}\|^2$$



- Why are these equivalent?
  - Use Pythagorean theorem.
  - Maximizing **blue** segment is the same as minimizing the **green**

PCA Covariance Matrix Interpretation

- Recall our first PC, maximized variance:

$$\max_{\mathbf{v}} \ \mathbf{v}^T \mathbf{X}\mathbf{X}^T \mathbf{v} \quad \text{s.t.} \quad \mathbf{v}^T \mathbf{v} = 1$$

- Constrained optimization
  - Recall our usual approach: Lagrangian + KKT conditions

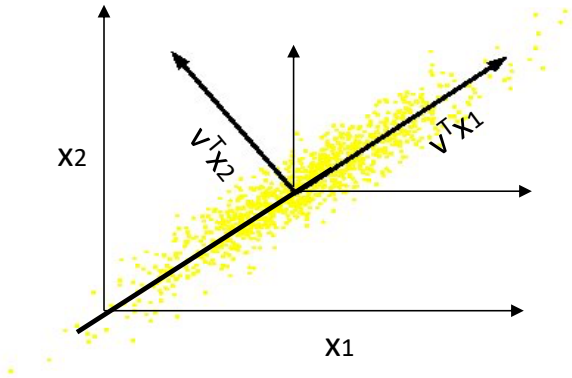
$$\text{Lagrangian: } \max_{\mathbf{v}} \mathbf{v}^T \mathbf{X}\mathbf{X}^T \mathbf{v} - \lambda \mathbf{v}^T \mathbf{v}$$

$$\partial / \partial \mathbf{v} = 0 \ \ (\mathbf{X}\mathbf{X}^T - \lambda \mathbf{I})\mathbf{v} = 0 \ \ \Rightarrow \boxed{(\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda \mathbf{v}}$$

PCA Covariance Matrix Interpretation

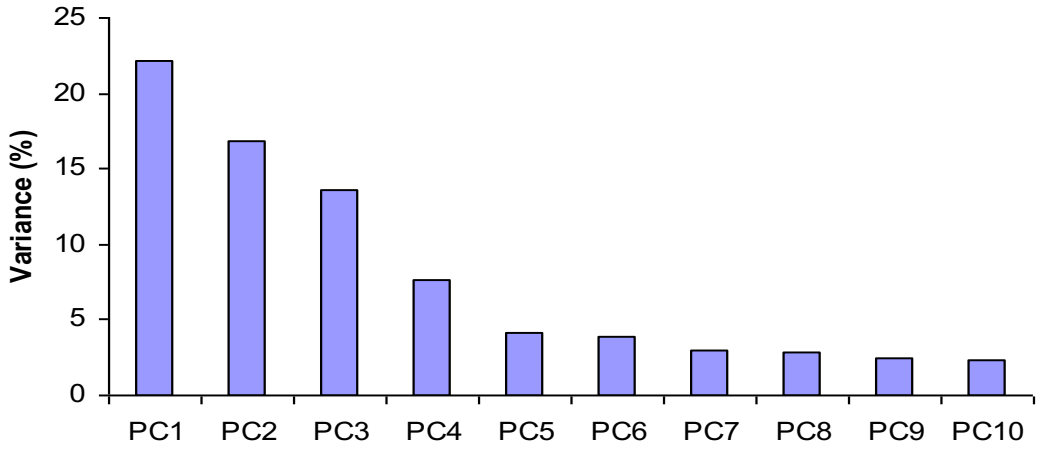
- So… $\Rightarrow \boxed{(\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda\mathbf{v}}$
- Means that v (the first PC) is an eigenvector of XX^T
- Its eigenvalue λ denotes the amount of variability captured along that dimension

- PCs are just the eigenvectors…
  - How to find them? Eigendecomposition
- Don't need to keep all eigenvectors
  - Just the ones for largest eigenvalues



PCA Dimensionality Reduction

- In high-dimensional problems, data sometimes lies near a linear subspace, as noise introduces small variability
- Only keep data projections onto principal components with **large** eigenvalues
- Can *ignore* the components of smaller significance.



Application: Image Compression

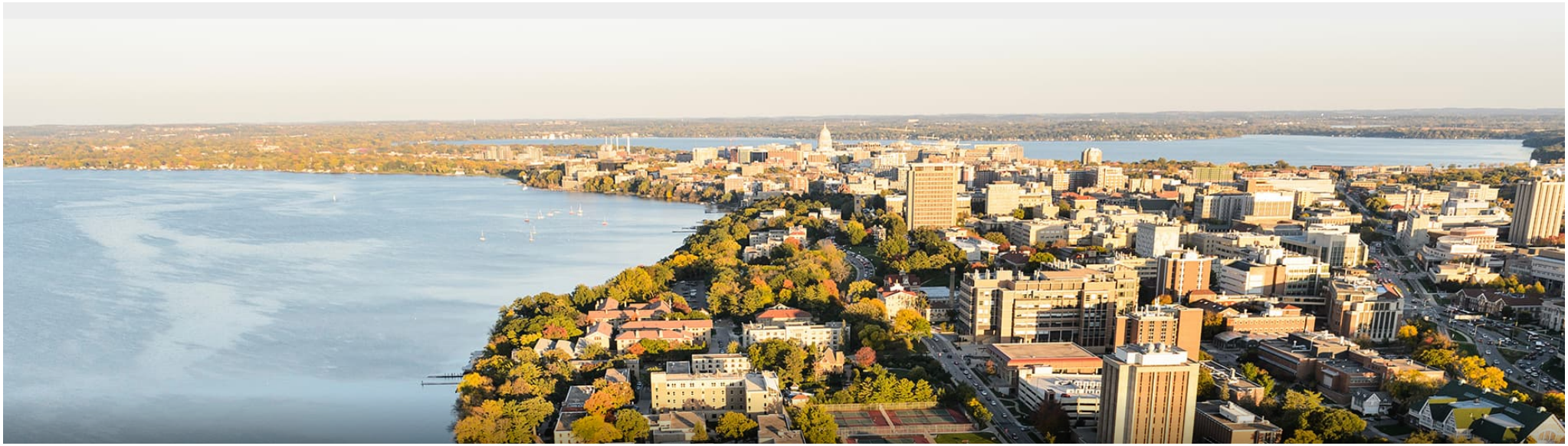
- Start with image; divide into 12x12 patches
  - I.E., 144-D vector
  - **Original image:**

Application: Image Compression

- Project to 6D,

Compressed

Original



Break & Quiz

Q1-1: Are these statements true or false?
(A) The principal component with the largest eigenvalue maximizes the reconstruction error.
(B) The dimension of original data representation is always higher than the dimension of transformed representation of PCA.

1. True, True
2. True, False
3. False, True
4. False, False

Q1-1: Are these statements true or false?
(A) The principal component with the largest eigenvalue maximizes the reconstruction error.
(B) The dimension of original data representation is always higher than the dimension of transformed representation of PCA.

1. True, True
2. True, False
3. False, True
4. False, False ⟵

(A) The principal component with the largest eigenvalue captures the maximum amount of variability which is equivalent to minimum reconstruction error.
(B) If the matrix XX^T is full-rank, they can be of the same dimension.

Outline

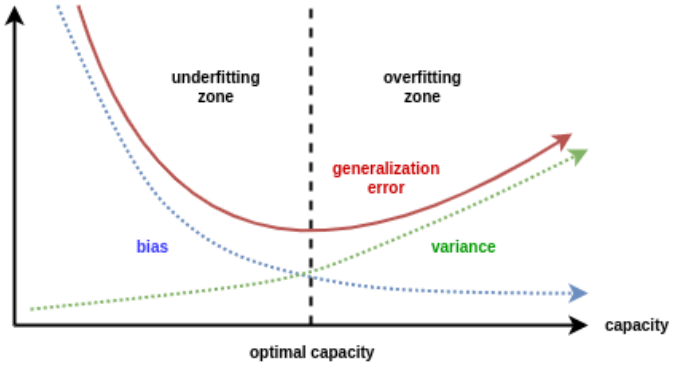
- **Review & PCA**
  - Intuition, operation, interpretations, compression
- **Intro to Learning Theory**
  - Error decomposition, bias-variance tradeoff
- **PAC Learning Framework**
  - Definition, intuition, sample complexity bounds

Learning Theory

- Goal: try to analyze error, and especially generalization
  - i.e., **the expected error** on the whole distribution

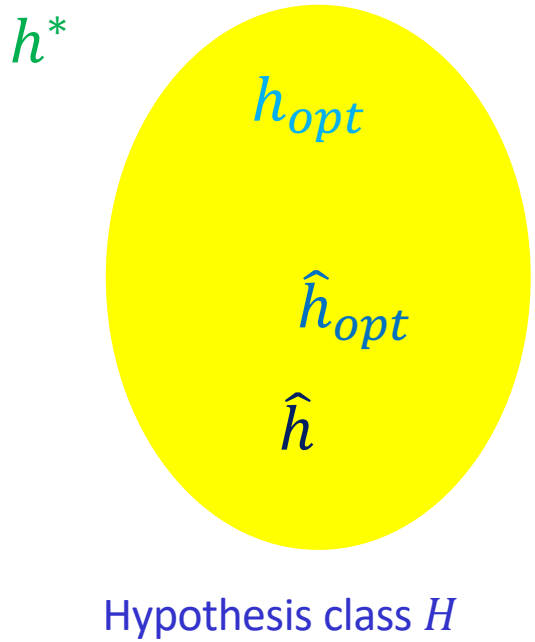
- We will cover a few ideas:
  - Error decomposition & generalization
  - Bias-variance tradeoff
  - PAC framework

- Deep subject overall.



Error Decomposition

- h^*: the optimal function (Bayes classifier)
- h_{opt}: the optimal hypothesis on the data distribution
- $\hat{h}_{opt}$: the optimal hypothesis on the training data
- $\hat{h}$: the hypothesis found by the learning algorithm



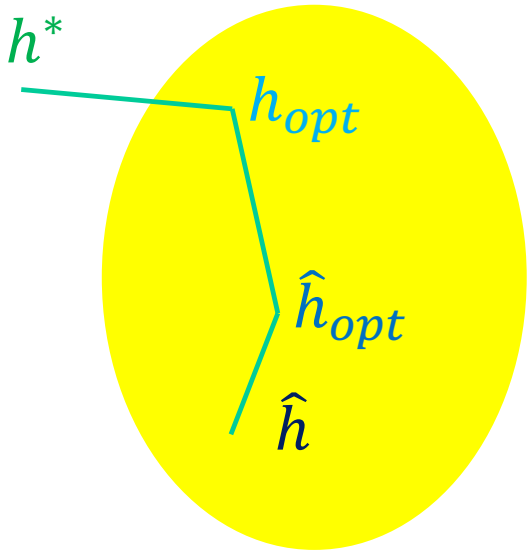
Error Decomposition

$$err(\hat{h}) - err(h^*)$$

$$= err(h_{opt}) - err(h^*)$$

$$+ err(\hat{h}_{opt}) - err(h_{opt})$$

$$+ err(\hat{h}) - err(\hat{h}_{opt})$$



Hypothesis class H

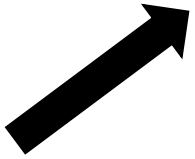
Error Decomposition

$$err(\hat{h}) - err(h^*)$$

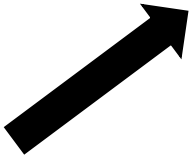
$$= err(h_{opt}) - err(h^*)$$

$$+ err(\hat{h}_{opt}) - err(h_{opt})$$

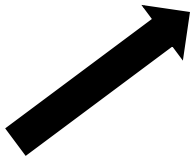
$$+ err(\hat{h}) - err(\hat{h}_{opt})$$



Approximation error
due to problem modeling (the choice of hypothesis class)



Estimation error
due to finite data



Optimization error due to imperfect optimization

Bounding Estimation Error

$$err(\hat{h}_{opt}) - err(h_{opt})$$

$$= err(\hat{h}_{opt}) - \widehat{err}(\hat{h}_{opt})$$

$$+ \widehat{err}(\hat{h}_{opt}) - err(h_{opt})$$

$$\leq err(\hat{h}_{opt}) - \widehat{err}(\hat{h}_{opt})$$

$$+ \widehat{err}(h_{opt}) - err(h_{opt})$$

$$\leq 2 \sup_{h \in H} |err(h) - \widehat{err}(h)|$$

Another Decomposition

$$err(\hat{h}) = \widehat{err}(\hat{h}) + \underbrace{[err(\hat{h}) - \widehat{err}(\hat{h})]}_{\text{Generalization gap}}$$

$$\leq \widehat{err}(\hat{h}) + \sup_{h \in H} |err(h) - \widehat{err}(h)|$$

- The training error $\widehat{err}(\hat{h})$ is what we can compute
- Need to control the **generalization gap.**
  - How?

Bounding the Generalization Gap

Have: $err(\hat{h}) \leq \widehat{err}(\hat{h}) + \sup_{h \in H} |err(h) - \widehat{err}(h)|$

- How do we deal with the right-hand term?
- Have, for example,

$$|err(h) - \widehat{err}(h)| \leq R(H) + \sqrt{\log\left(\frac{1}{\delta}\right)/2n}$$

for all h in H and where n is the number of samples, R(H) is the **Rademacher complexity** of the function class

Bounding the Generalization Gap

$$|err(h) - \widehat{err}(h)| \leq R(H) + \sqrt{\log\left(\frac{1}{\delta}\right)/2n}$$

for all h in H and where n is the number of samples, R(H) is the **Rademacher complexity** of the function class

- Rademacher complexity: a measure of how "large" the hypothesis is.
  - How much random data can it fit?
  - Other versions: VC complexity, Gaussian complexity

Bias-Variance Tradeoffs

Consider the task of learning a regression model given a training set $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$

- A natural measure of the **error** of f is

$$E_D[(y - f(\mathbf{x};\ D))^2]$$

  - Expectation is taken with respect to the real-world distribution of instances (not the empirical one)

Bias-Variance: Derivation

Take a fixed $\mathbf{x}$. Can rewrite:

$$E_D[(y - f(\mathbf{x};\ D))^2] =$$

$$\underbrace{E_D[(y - E[y|\mathbf{x}])^2]}_{\text{Variance of y given x (unrelated to model)}} + \underbrace{(f(x; D) - E[y|x])^2}_{\text{Error of f as a predictor}}$$

Bias-Variance: Derivation

Let's look at the 2nd term, and take the expectation over datasets:

$$E_D[(f(\boldsymbol{x}; D) - E[y|\boldsymbol{x}])^2] =$$
$$(E_D[f(\boldsymbol{x}; D)] - E[y|\boldsymbol{x}])^2 + ED[(f(\boldsymbol{x}; D) -$$
$$ED[f(\boldsymbol{x}; D)]^2] =$$

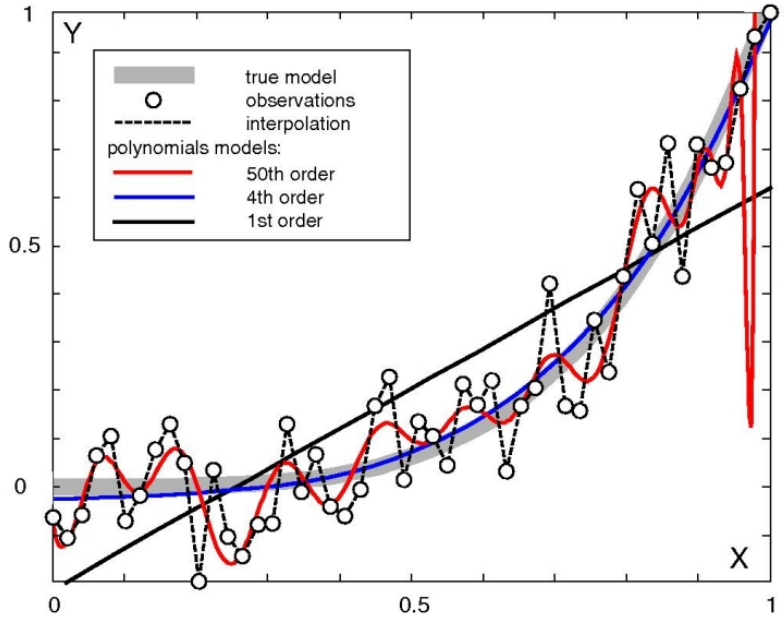
Bias

Variance

- **Bias**: if on average $f(\boldsymbol{x}; D)$ differs from $E[y \mid \boldsymbol{x}]$ then $f(\boldsymbol{x}; D)$ is a biased estimator of $E[y \mid \boldsymbol{x}]$
- **Variance**: $f(\boldsymbol{x}; D)$ may be sensitive to D and vary a lot from its expected value

Bias-Variance: Polynomial Interpolation

- **Example**:
  - 1st order polynomial has high bias, low variance
  - 50th order polynomial has low bias, high variance
  - 4th order polynomial represents a good trade-off

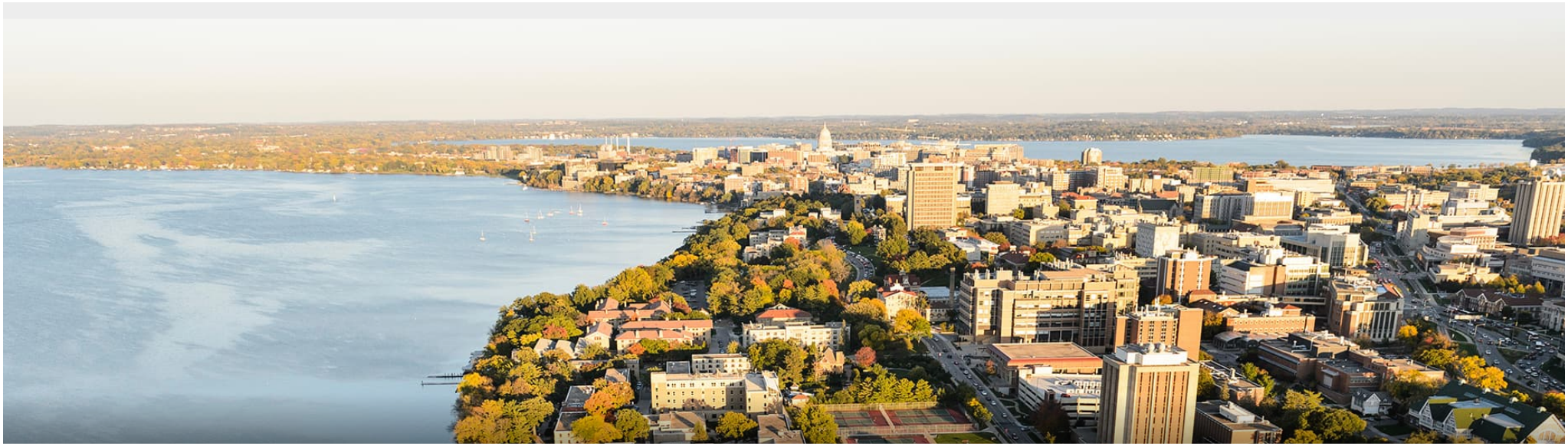


Bias-Variance: Idea

Predictive error has two controllable components

- expressive/flexible learners reduce *bias*, but increase *variance*

- For many models we can trade-off these two components (e.g. via our selection of k in k-NN)
- The optimal point in this trade-off depends on the particular problem domain and training set size
- Not necessarily a strict trade-off; e.g. with ensembles we can often reduce bias and/or variance without increasing the other term



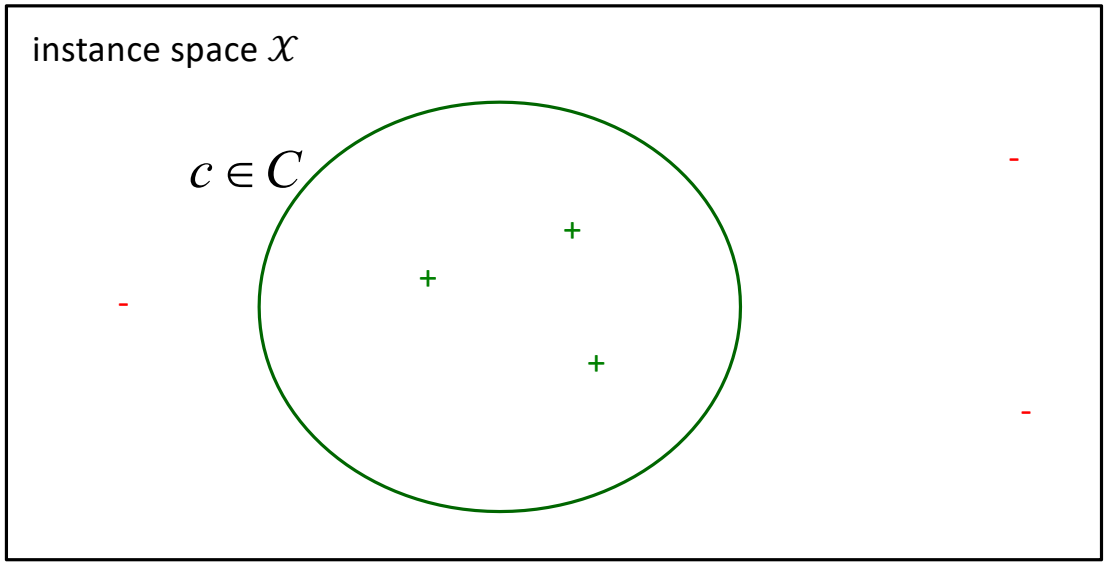
Break & Quiz

Outline

- **Review & PCA**
  - Intuition, operation, interpretations, compression
- **Intro to Learning Theory**
  - Error decomposition, bias-variance tradeoff
- **PAC Learning Framework**
  - Definition, intuition, sample complexity bounds

PAC Learning Setup

PAC learning is a framework used for theoretical analysis. Basic setting:



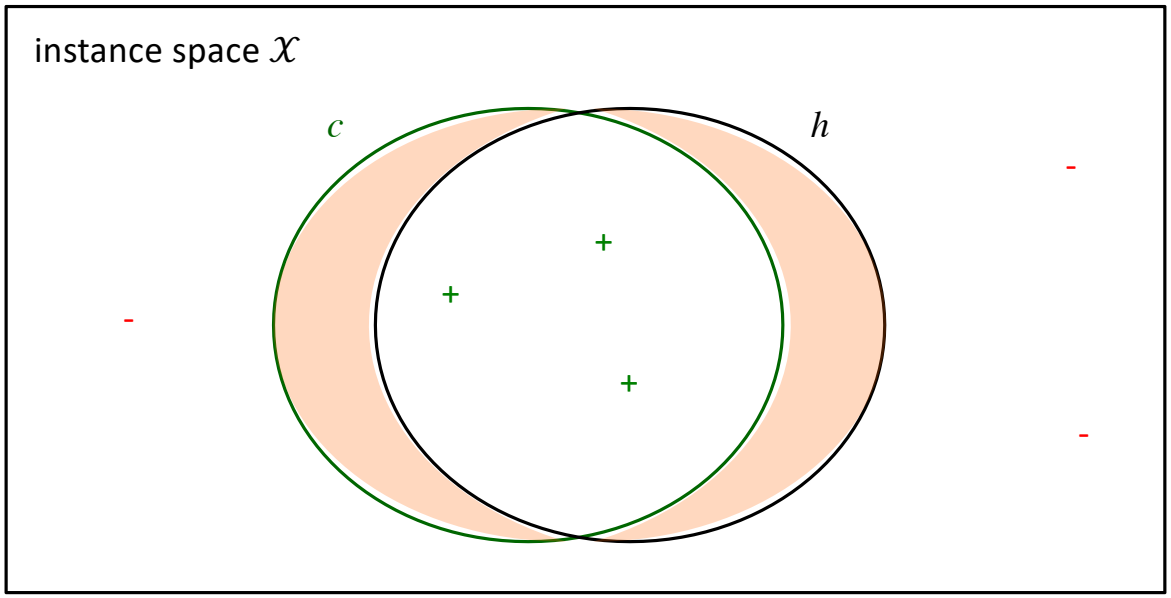
- Set of instances $\mathcal{X}$
- Set of hypotheses (models) H
- Set of possible target concepts C
- Unknown probability distribution $\mathcal{D}$ over instances

PAC Learning Setup

We get a set D of training instances $(\boldsymbol{x}, c(\boldsymbol{x}))$ for some target concept c in C

- each instance $\boldsymbol{x}$ is drawn from distribution $\mathcal{D}$
- class label $c(\boldsymbol{x})$ is provided for each $\boldsymbol{x}$

- learner outputs hypothesis h modeling c
- *Goal:* the *true error* of hypothesis h refers to how often h is wrong on future instances drawn from $\mathcal{D}$



PAC Learning: Two Error Types

We have **two** kinds of errors:

True error: (i.e., on any instance from distribution d):

$$error_{\mathcal{D}}(h) \equiv P_{\mathcal{D}}[c(x) \neq h(x)]$$

Empirical error: (I.e., on our dataset)

$$error_{D}(h) \equiv P_{x \in D}[c(x) \neq h(x)] = \frac{\sum_{x \in D} \delta(c(x) \neq h(x))}{|D|}$$

Goal: Can we bound $error_{\mathcal{D}}(h)$ in terms of $error_{\mathrm{D}}(h)$?

PAC Learning Definition

Consider a class C of possible target concepts defined over a set of instances $\mathcal{X}$ of length n, and a learner L using hypothesis space H

- C is **PAC learnable** by L using H if, for all $c \in C$, distributions $\mathcal{D}$ over $\mathcal{X}$, ε such that $0 < \varepsilon < 0.5$, δ such that $0 < \delta < 0.5$,

- The learner L will, with probability at least $(1\text{-}\delta)$, output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \varepsilon$ in time that is polynomial in the quantities:

$$1/\varepsilon \ , 1/\delta, n, \text{size}(c)$$

"**Probably Approximately** Correct"

PAC Learning Applications

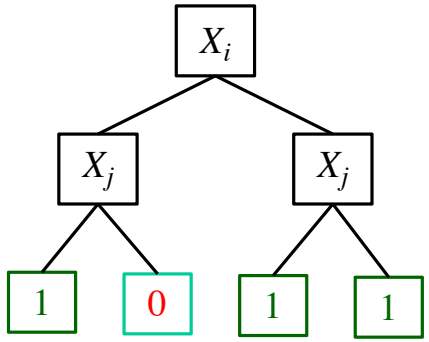
For finite hypothesis classes, the sample complexity (i.e., the m) so that we get a learner that satisfies the above definition is

$$m \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

Error tolerance

Size of hypothesis class

Probably correct



Can apply to, for example, decision trees of depth 2 for binary feature vectors

- |H| is the number of splits (ie, n choose 2 times 16: # split choices times # leaf labelings)
- For probability ≥ 0.99 with error ≤ 0.05, number of samples we need is:
- Example: for $n=100$, $m \geq 318$

$$m \geq \frac{1}{.05}\left(\ln\left(8n^2 - 8n\right) + \ln\left(\frac{1}{.01}\right)\right)$$

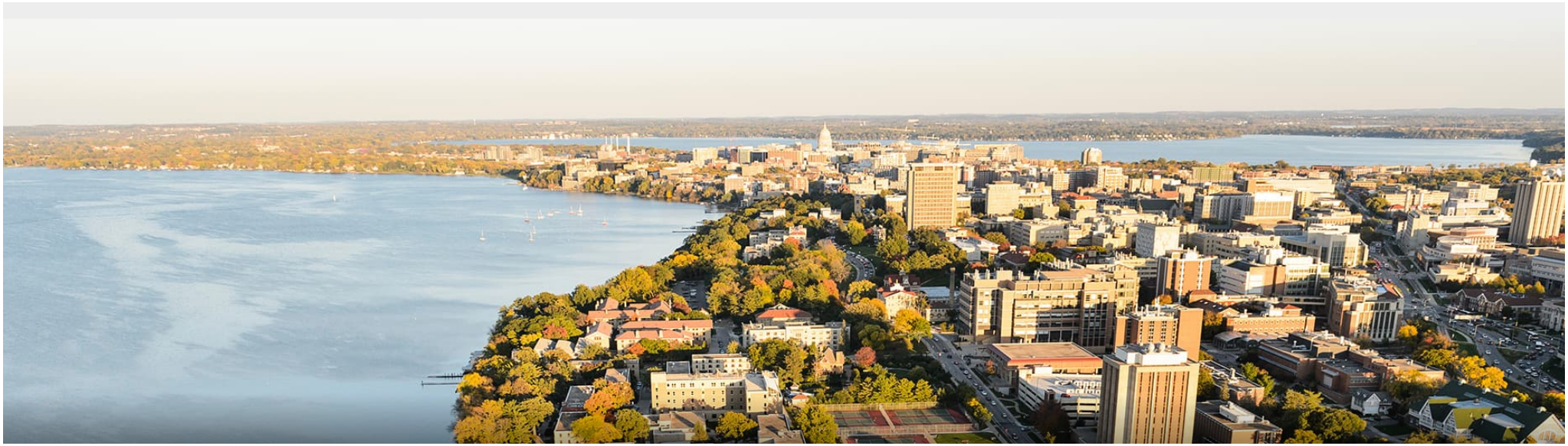
PAC Learning Discussion

PAC formalizes learning task, allows for non-perfect learning (indicated by ε and δ)

- Requires polynomial computational time

- PAC analysis has been extended to explore a wide range of cases
  - the target concept not in our hypothesis class
  - infinite hypothesis class (VC-dimension theory)
  - noisy training data
  - learner allowed to ask queries
  - restricted distributions (e.g. uniform) over $\mathcal{D}$

- Most analyses are worst case
- Sample complexity bounds are generally not tight



Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov, Fred Sala